Supporting Information

Effect of Environmental Conditions on the Permeability of High Density Polyethylene Film to Fumigant Vapors

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Model including plastic film and water film in series

To mathematically describe the physical system, three differential equation are needed. One describes the change in concentration of fumigant in the source chamber, one describes fumigant movement and partitioning in the water film and the third describes changes in fumigant concentration in the receiving chamber. Mathematically, these differential equations are

$$\begin{aligned} \frac{\partial C_s}{\partial t} &= -\frac{J_s}{L_s} \\ \frac{\partial C_w}{\partial t} &= D_w \frac{\partial^2 C_w}{\partial x^2} \\ \frac{\partial C_r}{\partial t} &= \frac{J_r}{L_r} \end{aligned} \tag{A1}$$

where $C_s(t)$ and $C_r(t)$, respectively, are gas-phase concentrations in the source and receiving chambers; $C_w(x,t)$ is the liquid-phase concentration in the water film and is related to gas-phase concentrations using $C_w = C_{gas}/K_h$; J_s and J_r are mass flux densities of the fumigant; and L_s, L_r and L_w, respectively, are the lengths of the source chamber, receiving chamber and water film. Mass conservation requires that the mass leaving the source chamber must enter the water film, and, mass leaving the water film must enter the receiving chamber. To solve A1, initial and boundary conditions are needed. At the start of the experiment, the initial fumigant concentration is zero everywhere except the source chamber where the concentration is C_o. To solve the equation for the water film requires two boundary conditions which couple this equation to the source and receiving chambers. They are

$$C_w(0,\ t) = \frac{C_s(t)}{K_h} .$$

$$-D_w \left.\frac{\partial C_w}{\partial t}\right|_{x=L_w} = h\left[C_w(L_w,\ t) - \frac{C_r(t)}{K_h} \right] \tag{A2}$$

The Equations A1 and A2 can be solved using Laplace Transforms (Haberman, 1983). Incorporating the initial and boundary conditions into A1, solving and rearranging gives the concentration in the water phase

$$C_w(x,\ t) = \frac{C_o L_s}{K_h (L_r + L_s) + L_w} + \\ 2\, C_o L_s \sum_{i=1}^{\infty} e^{-D_w k_n^2 t} \left\{ A_n\, Cos[k_n(L_w - x)] + B_n\, Sin[k_n(L_w - x)] \right\} \tag{A3}$$

with

$$A_n = \frac{h - D_w K_h k_n^2 L_r}{\xi\, Cos[k_n L_w] - \zeta\, Sin[k_n L_w]} \\ B_n = \frac{-h K_h k_n L_r}{\xi\, Cos[k_n L_w] - \zeta\, Sin[k_n L_w]} \tag{A4}$$

and

$$\begin{aligned} \xi &= -D_w K_h k_n^2 L_r \left(4 K_h L_s + L_w\right) + h\left\{L_w + K_h\left(2(L_r + L_s) - K_h k_n^2 L_r L_s L_w\right)\right\} \\ \zeta &= D_w K_h k_n L_r \left(3 - K_h k_n^2 L_s L_w\right) + h\left\{K_h k_n\left(3 K_h L_r L_s + (L_r + L_s) L_w\right) - \frac{1}{k_n}\right\} \end{aligned} \qquad \text{(A5)}$$

The concentrations in the source and receiving chamber, respectively are

$$C_s(x,\ t) = K_h\, C_w(0,\ t) \qquad \text{(A6)}$$

$$C_r(x,\ t) = \frac{C_o K_h L_s}{K_h (L_r + L_s) + L_w} + 2\, C_o L_s K_h\, h \sum_{i=1}^{\infty} \frac{e^{-D_w k_n^2 t}}{\xi\, Cos[k_n L_w] - \zeta\, Sin[k_n L_w]} \qquad \text{(A7)}$$

The k_n's are values for which the following equation yields zero

$$\begin{aligned} &K_h k_n \left(D_w K_h k_n^2 L_r L_s - h(L_r + L_s)\right) Cos\left(k_n L_w\right) + \\ &\quad \left(D_w K_h k_n^2 L_r + h(K_h^2 k_n^2 L_r L_s - 1)\right) Sin\left(k_n L_w\right) = 0 \end{aligned} \qquad \text{(A8)}$$

References

Haberman, R., 1983. *Elementary applied partial differential equations with Fourier series and boundary value problems*, Prentice-Hall, New Jersey, 533 pp.